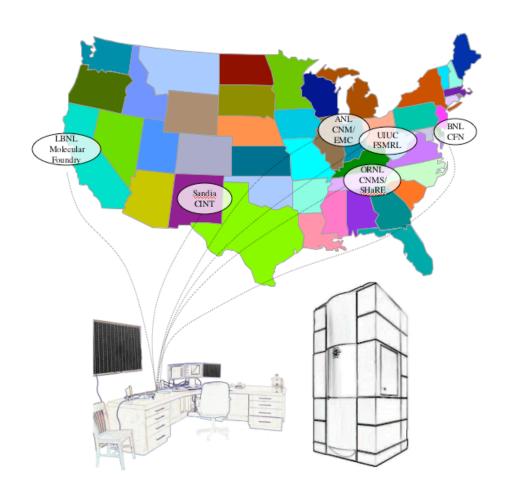
WORKSHOP REPORT

EXTENDING THE TEAM CONTROL ROOM

WORKSHOP ON REMOTE ACCESS TO THE TRANSMISSION ELECTRON ABERRATION-CORRECTED MICROSCOPE







PROGRAM

Monday, 23rd of June 2008—Bldg. 62 203 –Leo Brewer Room

8:30 am	Welcome, TEAM overview and workshop goals Ulrich Dahmen
8:55 am	TEAM project status
9:20 am	CNMS overview and needs for advanced microscopyLinda Horton*
9:45 am	COFFEE
10:15 am	Foundry overview and needs for advanced microscopy Jim De Yoreo
10:40 am	Electron microscopy and nano-science at ANL: new opportunities through TEAM
11:05 am	In situ electron microscopy enabled by a TEM-SPM platform at CINTJianyu Huang
11:30 am	Overview and needs for electron microscopy at CFN Lihua Zhang
11:55 am	LUNCH
1:00 pm	The SHaRE user facility and microscopy at ORNLKarren More*
1:25 pm	TEAM stage: opportunities for in-situ microscopy Ivan Petrov
1:50 pm	TEAM stage: prospects for remote operations Thomas Duden
2:15 pm	Driving TEAM remotely: operations, alignments, feasibilityRolf Erni
2:40 pm	COFFEE and TEAM VISIT
3:25 pm	TEAM software
3:45 pm	ESnet Eli Dart
4:10 pm	Practical aspects and requirements of remote microscopy operation for research oriented applications
4:35 pm	Remote microscopy at FEI: "Brains unite" part II Auke van Balen
5:00 pm	DiscussionNestor Zaluzec

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^{*} Unable to attend due to unforeseen circumstances.

INTRODUCTION

The prospect of remote access to the TEAM microscopes at Department of Energy microscopy laboratories that are co-located with Nanoscience Facilities was an important part of the original driving force for the TEAM project. To prepare this capability the project aims to enable other institutes to set up portals that can connect remotely to the TEAM microscope. By establishing software, network and hardware requirements for the partner labs, the project is laying the foundation to make TEAM's unique capabilities available to the broader scientific community. Due to the intrinsic complexity of the TEAM instruments and for the specific advanced experiments that will require the use of their unprecedented capabilities, network bandwidth is a critical limitation to seamless remote operability. With high-speed data transfer, operating the machine from the partner laboratories could be identical to operating it from Berkeley, bringing to bear in full the collaborative nature of the project. Hence the idea of enabling "access portals" at participating National Laboratories, linked to TEAM through a high performance network line such as that provided by ESnet, a Department of Energy – Office of Science facility specifically created to support those aspects of DOE science that depend on high performance networking for success.

However, to make broad user access to the TEAM instrument via high-bandwidth remote portals a reality, the specific challenges of this new mode of operation must be fully understood. This workshop was thus organized with a view to explore the scientific needs, mechanics and logistics for remote access to the TEAM instrument after it starts users operations in 2009, with the eventual goal to formulate a plan for "extending the TEAM control room" to the partner laboratories. In addition to the National Center for Electron Microscopy (NCEM), ESnet and TEAM commercial partners FEI Company, the concerned laboratories include: the Center for Nanoscale Materials and Electron Microscopy Center at Argonne National Laboratory (CNM and EMC, ANL), the Center for Functional Nanomaterials at Brookhaven National Laboratory (CFN, BNL), the Center for Nanophase Materials Sciences and the Shared Research Equipment program at Oak Ridge National Laboratory (CNMS and SHaRE, ORNL), the Center for Integrated Nanotechnologies at Sandia National Laboratories (CINT, Sandia), the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign (FSMRL, UIUC) and the Molecular Foundry at the Lawrence Berkeley National Laboratory.

After an update on the project status and the plans for start of users operations for TEAM 0.5, the first double-corrected TEAM column, the major focus was therefore on identifying opportunities and scenarios for actual research via remote TEAM operations. Participants from partner laboratories were encouraged to present an overview of the scientific research carried out at their respective institutions, along with a description of the current capabilities and anticipated needs for advanced electron microscopy. Their views and outlines of specific projects, types of experiments or modes of operation that would benefit from remote TEAM access are paramount, since the remote "portals" must

be tailored to suit specific scientific needs. As discussed in the technical session of this workshop, it is essential to define accurately software, hardware and support requirements for remote operations as well as ensure the compatibility of remote control with different techniques of microscopy. Only then can the capabilities of ESnet and the proposed remote interface be exploited fully.

PAVING THE WAY FOR REMOTE TEAM OPERATIONS

The sheer variety of perspectives demonstrated by the participants toward the goal of remote operations of the TEAM microscope made for an invaluable and comprehensive discussion. Scientific, technical and operational aspects were all considered and provided essential guidance toward making remote TEAM operations a reality.

Expert remote operators

Four main modes of remote operations were identified:

- *1. remote observer*: observes and recommends actions to the actual non-remote operator. This mode is most suitable for infrequent, one-time or first-time users.
- 2. remote controller: a remote user directs, controls and finishes a measurement that was set-up and started by a non-remote operator. This mode would be suitable for frequent users with limited experience.
- 3. remote operator: runs measurements fully by her/himself, without any non-remote support. This mode requires the greatest level of training and skill and would be most suitable for a repeat/follow up experiment after on-site use of the microscope.
- 4. remote expert: a remote operator takes brief control of the machine to perform specific action of which she/he has a specific expertise, thus assisting a non-remote user. This mode is suitable for very advanced tasks, and brings the multi-laboratory collaboration to full bear.

Whilst all modes have advantages and drawbacks, a consensus was reached on the most efficient use of remote capabilities. In many respects, extending the microscope control room to a remote location involves a significant increase in the degree of complexity for both the operator and the local support staff. Remote control must therefore be reserved for cases where it increases the available microscope time, whilst saving some significant travel burden. Of the four aforementioned modes, the remote operator and remote expert modes seem to suit these conditions best. An important corollary is that expert TEAM operators must be available at the partner Laboratories for the early implementations of remote operations. Extensive discussions at this workshop identified the optimum initial link with Argonne National Laboratory where ESnet connections are most readily established and subsequently with Oak Ridge National Laboratory. Both locations have expert users of TEAM-like instruments and an infrastructure to support external user research in electron beam microcharacterization.

Local technical optimization

From a technical point of view, the importance of liaising with the IT department of the future remote portals was strongly emphasized: ESnet provides high-bandwidth network connectivity between the various National Laboratories, but the network structure at the portal ends must also be mastered and optimized.

The following recommendations were thus put forth:

- 1. Involve network engineers at the partner laboratories very early in the implementation of remote operations.
- 2. Identify a test site for early high-bandwidth networking tests. Due to considerable past experience with various aspects of remote microscopy and existing links with the networking department and ESnet at LBNL, Argonne National Laboratory was identified as a likely site for such purposes.
- 3. Start testing the data transfer capabilities with "dummy" data streams, akin to what is customary in the field of high energy physics (connectivity to/from the LHC in Geneva for instance has been undergoing years of tests with non-scientific data).

Test remote experiment

A key recommendation was agreed upon by all participants in the open discussion scheduled at the end of the workshop discussion. The technical ability and expertise to create remote TEAM portals are readily available: as the enthusiasm expressed by all workshop participants clearly demonstrated, these portals would service a real scientific need.

The first step to make those portals a reality must however be the formulation of a specific test experiment that meets all aforementioned criteria: operator expertise, networking capabilities of the remote site, necessity for remote operation... In particular, this experiment would in a first step be carried out on site at NCEM, by an expert operator from one of the partner laboratories and would then be repeated entirely remotely.

The type of experiment chosen will determine many critical aspects of the initial implementation of remote operations: size of the data stream to be set up, level of complexity of the additional remote interface, expertise and training of the operator. Once these parameters are set up, they will provide the building blocks for the more comprehensive remote control room, which the present workshop helped outline.

SUMMARY

The most important conclusion from this workshop was the consensus that remote operation should be driven by scientific needs, and that the best way to establish these needs is by providing a broadband link and facilitating initial high-level experiments. Making use of the existing infrastructure at the partner labs, the expertise of advanced users and staff, as well as the secure environment provided by the framework of a connection between national laboratories, this initial experience will guide further developments. Remote access thus becomes a process of evolution and learning rather than a rigid pre-defined framework. It is expected that the solutions for specific issues

such as bandwidth, local support, scientific environment, security, user interface and proposal review will evolve rapidly and in response to needs that become apparent during testing and use of the remote access portals. The approach developed in this workshop builds on existing infrastructure while leaving maximum flexibility for other institutions to establish remote portals that truly "extend the TEAM control room" to all of the Nanoscience Centers and partner labs.

CONTRIBUTED ABSTRACTS

Welcome, TEAM overview and workshop goals

U. Dahmen, NCEM, Lawrence Berkeley National Laboratory

The TEAM project opens many new possibilities for nanoscale research and discovery by redesigning the electron microscope around aberration correction in a collaborative effort that involves several DOE and commercial partners. The underlying vision is the idea of providing a sample space for electron scattering experiments in a tunable electron optical environment by removing some of the constraints that have limited electron microscopy until now. The resulting improvements in spatial, spectral and temporal resolution and the possibility of exotic electron-optical settings will enable new types of experiments. After its completion at NCEM in 2009, the instrument will be made available to the scientific user community. Although most of the operation of the TEAM instrument is expected to take place on site, the long-term goal is to make the instrument available via remote operation. This workshop will examine the needs and opportunities for broadband remote operation of TEAM from select locations at National Labs and nanoscience centers.

TEAM project status

P. Denes, Lawrence Berkeley National Laboratory

TEAM is a Department of Energy 20 Year Facilities Roadmap project to develop a best-in-class electron scattering instrument that supports the identified needs of the U.S. research community and the DOE mission. The TEAM microscope aims to enhance the capabilities of the existing Electron Beam Microcharacterization Centers as well as the collocated DOE Nanoscale Science Research Centers, and one of the ways these enhanced capabilities will come about is through remote operation. TEAM is being delivered in a staged fashion, with an initial instrument, TEAM 0.5 – which already delivers 0.5Å spatial and 0.1 eV energy performance – to be replaced by the final TEAM I microscope, which will add chromatic aberration correction. The current status of the TEAM project will be presented.

CNMS overview and needs for advanced microscopy

Linda L. Horton, Center for Nanophase Materials Sciences. Oak Ridge National Laboratory

The Center for Nanophase Materials Sciences (CNMS), one of DOE's new nanoscience user facilities, offers a wide range of capabilities to the user community including advanced synthesis, characterization, and theory/modeling. CNMS had over 300 users last fiscal year, with all indications that there will be an increase for FY2008. Among the

most widely used tools for characterization are the electron microscopes – about half of the user projects include advanced electron microscopy or scanning probes. CNMS has a partner relationship with ORNL's Shared Research Equipment program to provide microscopy to the combined user community. This presentation will discuss the needs for advanced microscopy as defined by the nanoscience user community. There is an emphasis on development of improved techniques for in situ microscopy and for measurement of properties combined with structure and chemistry.

Molecular Foundry overview and needs for advanced microscopy

J. De Yoreo, Molecular Foundry, Lawrence Berkeley National Laboratory

The six facilities of the Molecular Foundry provide Users with capabilities and expertise for synthesis of novel inorganic, organic and biological nanostructured building blocks, measurement and simulation of their properties, and their integration into complex assemblies. The research themes of the Foundry's internal research program target combinatorial synthesis of nanomaterials, "single digit" nanofabrication, interfaces in nanomaterials, and multimodal *in situ* imaging and spectroscopy. While electron microscopy plays a significant role in the characterization of nanostructures produced in all of its facilities, the Foundry is also working to make it a routine method for investigating catalysis, assembly, and structural evolution through *in situ* imaging in both gas and fluid phases. In particular, the application of *in situ* imaging to soft materials and hard/soft interfaces is emerging as a major focus of our effort to develop new tools and techniques for the NSRC User community.

Electron microscopy and nanoscience at Argonne: new opportunities through TEAM

Dean Miller, Argonne National Laboratory

Electron microscopy and scattering play a key role in materials research and, especially, in studies of nanoscale materials and nanoscale phenomena. The Electron Microscopy Center serves as the focal point for electron microscopy and scattering at Argonne and has close partnership with the Center for Nanoscale Materials to help meet the microscopy needs for their user communities. While the Electron Microscopy Center offers expertise and a wide range of microscopy capabilities, remote control of TEAM offers the possibility to provide local users with access to a world-class instrument with capabilities that are not available elsewhere. Many of the emerging scientific opportunities within the Center for Nanoscale Materials require atomic scale resolution, increased analytical sensitivity, smaller probes with high beam current and ultra-high stability. TEAM offers many of these capabilities and, through remote control, the opportunity to make these capabilities available to an even broader user community. In this talk, some of the scientific opportunities made possible through TEAM will be presented and some of the challenges to making those capabilities available through remote operation of TEAM will be discussed.

In situ electron microscopy enabled by a TEM-SPM platform at CINT

Jianyu Huang, Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories

Transmission electron microscopy (TEM) is a powerful tool for structural characterization of materials. However *in-situ* studies of the mechanical, electrical and thermal properties of materials at a nanometer scale are still challenging. A scanning probe microscopy (SPM), including scanning tunneling microscopy (STM), atomic force microscopy (AFM), and nano-indentor, explores the physical and mechanical properties of materials down to a single atom level but without internal structural information. A combined TEM-SPM platform, which integrates a fully functional SPM into a TEM, takes advantage of both the SPM and the TEM capabilities and provides unprecedented opportunities to probe the structural, mechanical, electrical, and thermal properties of materials *in-situ* down to a nanometer scale.

This allows for direct correlation of the physical and mechanical properties to the atomic-scale microstructure. In this talk, I will review our recent progress in using the TEM-SPM platform to probe the electrical and mechanical properties of carbon nanotubes [1]. First, individual multiwall carbon nanotubes are peeled off layer-by-layer by electric breakdown inside the TEM. This provided new insights into the transport property of nanotubes. Second, plastic deformation, such as superplasticity, kink motion, dislocation climb, and vacancy migration, was discovered in nanotubes for the first time. Emerging directions of using the TEM-SPM platform and the needs for aberration-corrected TEM to conduct cutting edge research in nanoscience and nanotechnology will be highlighted.

[1] J.Y. Huang *et al.*, Nature 439, 281 (2006); J.Y. Huang *et al.*, Phys. Rev. Lett. 94, 236802 (2005); 97, 075501 (2006); 98, 185501 (2007); 99, 175593 (2007); 100, 035503 (2008).

Overview and needs for electron microscopy at CFN

Lihua Zhang, Eli Sutter, Joe Wall and Yimei Zhu, Center for Functional Nanomaterials, Brookhaven National Laboratory

The Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory provides state-of-the-art capabilities for synthesis, characterization, measurement, and theory of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions. The electron microscopy facility at CFN focuses on identifying nanoscale structure-property relationships of energy related materials by employing state-of-the-art instruments. We emphasize technique development that will enhance our facility capabilities for user based science as well as our own research projects. Currently, we have three TEMs at CFN: the JEOL2100F, the Hitachi HD2700C STEM with a probe corrector and the FEI Titan Environmental-TEM with an image corrector. Although these instruments provide a wide range of capabilities including high-resolution imaging, diffraction and spectroscopy as well as in-situ microscopy, very often the special, time and energy resolution of these instruments were not sufficient to meet our need. The TEAM instrument at LBL is a land mark microscope with

unprecedented resolutions and capabilities. As one of the five original participants in the TEAM project, we BNL scientists are eager to have access to the instrument. Our detailed needs for the TEAM instrument will be discussed in the presentation.

Electron microscopy at ORNL and in the ShaRE program

Karren More, ShaRE User Facility, Oak Ridge National Laboratory

The Shared Research Equipment (SHaRE) User Facility at Oak Ridge National Laboratory (ORNL) is one of three Electron Beam Microcharacterization Centers sponsored by the DOE's Office of Basic Energy Science, Division of Scientific User Facilities. This user facility houses a unique collection of advanced microscopes, including three FEG-TEM/STEMs, three FEG-SEMs, two dual-beam FIB systems, a LEAP, and an XPS. The facility supports user research in a variety of material's disciplines and is also the microscopy facility that supports users conducting research at ORNL's Center for Nanophase Materials Science (CNMS). The SHaRE facility (in collaboration with the HTML User Center) has previous experience with remote access on two TEM/STEM instruments, the Hitachi HF-3300 and the JEOL 2200FS, and the procedures for remote operation of these instruments will be discussed.

TEAM stage: opportunities for *in-situ* microscopy

Ivan Petrov, Eric Olson, and Todor Donchev, Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana

We are developing an enhancement of the TEAM stage that will combine the piezoelectric motors, position sensing, and stability of the beta module with the ability to do *in-situ* experimentation based on the application of electrical bias across, and current through, the sample. The stage will use a rotatable sample cartridge that can accommodate a standard 3 mm grid or an *in-situ* device with this diameter. In order to perform experiments and optimize the *in-situ* design, a prototype side-entry piezo stage with position encoding was fabricated and can operate in conventional TEMs. The side entry stage will be useful for preliminary experiments and troubleshooting before users book time on the TEAM instrument. We present experiments done using two microfabricated devices. First, a silicon nitride membrane based device developed at FS-MRL. Second, heating up to 1100°C and the melting of Au nanoparticles is demonstrated using a device made by Protochips. Other feasible experiments include the *in-situ* biasing of a samples, e.g. nanotubes or nanowires, the activation of a piezoelectric element, etc.

TEAM stage: prospects for remote operations

Thomas Duden NCEM, Lawrence Berkeley National Laboratory

The current TEAM stage controller has a TCP/IP based command interface. From the technical viewpoint, the remote control of the TEAM stage is trivial and has been tested to work from various off-site locations including e.g. Germany. The involved components are a specialized software containing LabVIEW and C++ parts that runs on

the remote host, and a suitable human interface device (HID). In contrast to the technical side, the distribution of software and hardware poses various issues that need to get addressed conceptually, including maintainability and security issues.

Driving TEAM Remotely - Operation, Alignments, Feasibility

Rolf Erni, NCEM, Lawrence Berkeley National Laboratory

In this presentation the feasibility of remotely operating the TEAM 0.5 microscope in its current configuration is discussed. We show the operation of TEAM 0.5 in the control room at NCEM and describe the different steps that define a microscope session, i.e., from aligning the microscope to storing the data. We discuss practical usability requirements of the (remote) software and the remote graphical user interface, the reliability of the hardware and what is actually demanded from the (remote) user. The presentation is intended to solve some of the issues that come up if one practically starts using TEAM 0.5 remotely; what can be done remotely and where are the limits, which steps unavoidably require on-site support at NCEM, and when is it beneficial to have what type of remote access to the microscope.

TEAM Software

Earl Cornell and Quentin Ramasse, NCEM, Lawrence Berkeley National Laboratory

Beyond the technological feat of breaking the 0.5 _ barrier, the TEAM project comprises a wealth of custom developments: the TEAM sample stage(s), discrete tomography techniques, advanced electron detectors... All these require a great deal of computer control as well as the ability to communicate seamlessly with the manufacturer's interface. A major effort is therefore underway to integrate all those software components and avoid producing an overly-complex, albeit functional, multi-application interface. This presentation will briefly outline the prospects of a unified software platform, designed with a view to provide all TEAM partners access to the new functionalities of the TEAM microscopes as well as the ability to add and integrate their own modules. In particular, the concept of a "super scripting language", reprising the existing microscope scripting capability and extending it to include the current developments (stage, detectors, remote operations), will be discussed.

ESNet

Eli Dart, ESNet, Lawrence Berkeley National Laboratory

ESnet is the high performance networking facility of the DOE office of science. ESnet's mission is to enable those aspects of DOE science that depend on high performance networking for success. I will discuss ESnet's current architecture - ESnet4 - and the network services that we provide in support of science and the Labs, and how the local networking organizations for the Labs connect to ESnet. I will also discuss what I expect

the networking for a TEAM portal might look like, and some possible ways that networking for TEAM portals might be achieved at remote sites.

Practical aspects and requirements of remote microscopy operation for researchoriented applications

Masashi Watanabe, NCEM, Lawrence Berkeley National Laboratory

Conventionally, users must visit facilities to conduct research in front of an instrument, otherwise users must commission local personnel to perform experiments by sending specimens with detailed descriptions if the users cannot be at the facilities. The latter case often causes several issues mainly due to miscommunication. Remote microscopy can be one of the ideal solutions for the facilities and users who locate far from the facilities. The fast speed internet lately available makes the remote operation possible. However, there are still several problems in the remote operation for research. Based on the author's limited experience [1], the remote operations require (1) intensive local supports at the facilities, (2) seamless interface for remote operation, and (3) remote users' local experience on the instrument. Despite of these issues, the remote-based research can open new possibilities for international scientific collaboration in the 21st century.

[1] Watanabe et al. Microsc. Microanal. 12(2006), Suppl.2, 534

Remote microscopy at FEI. Brains unite, part II: How do we get something that works?

A. van Balen, FEI Company

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